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ABSTRACT

<u>Discovery and Identification of Dimethylsilanediol as a Contaminant in ISS Potable</u> Water

In September of 2010, analysis of ISS potable water samples was undertaken to determine the contaminant responsible for a rise in total organic carbon (TOC). As analysis of the routine target list of organic compounds did not reveal the contaminant, efforts to look for unknown compounds was initiated, resulting in an unknown peak being discovered in the gas chromatography/mass spectrometry (GC/MS) analysis for glycols. A mass spectrum of the contaminant was then generated by concentrating one of the samples by evaporation and analyzing by GC/MS in full-scan mode. Although a computer match of the compound's identity could not be obtained with the instrument's database, a search with a more up to date mass spectral library yielded a good match with dimethylsilanediol (DMSD). Inductively Coupled Plasma/Mass Spectrometry (ICP/MS) analyses showed abnormally high silicon levels in the samples, confirming that the unknown contained silicon. DMSD was then synthesized to confirm the identification and provide a standard to develop a calibration curve. Further confirmation was provided by external Direct Analysis in Real Time (DART) GC/MS analysis. A preliminary GC/MS method was then developed and archived samples from various locations on ISS were analyzed to determine the extent of the contamination and provide data for troubleshooting. This paper describes these events in more detail as well as problems encountered in routine GC/MS analyses and the subsequent development of high performance liquid chromatography and LC/MS/MS methods for quantitation of DMSD.

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